Probing structure and energetics of proton-bound complexes N_2…HCO^+ and N_2H^+…OC using computational chemistry methods

Antonio Barrios, Dalton Boutwell, Onyi Okere, Monique Olocha, Oluwaseun Omodemi, Alexander Toledo, Martina Kaledin

N_2…HCO^+ and N_2H^+…OC are predicted to exist in interstellar clouds. These complexes involve HCO^+ and N_2H^+ fragments that are bound to N_2 and CO, respectively using hydrogen-bonded interaction. The reason these molecules are important is that the existence of nitrogen can be measured indirectly through ion-molecular complexes studied in this work. The measured vibrational spectra of molecules is an excellent way to characterize and detect molecules. We used B3LYP, MP2, and CCSD(T) computational methods to predict the structure and vibrational frequencies of N_2…HCO^+ and N_2H^+…OC and their fragments. The aug-cc-pVDZ and aug-cc-pVTZ basis sets were used. The stability of the complexes was described in terms of dissociations energies D_e and their zero-point energy (ZPE) corrected values, D_o. Both molecular complexes exhibit a linear geometry. Vibrational frequencies were obtained using normal mode analysis. The N_2H^+…OC proton transfer vibrations occur at around 1800 – 1900 cm^{-1}. H^+ bound within HCO^+ exhibit C-H vibration at ~2500-2700 cm^{-1}. The N_2…$HCO^{+\cdot}$ complex is more stable than N_2H^+…OC by ~7000 cm^{-1}. The ZPE corrected values for dissociation energies, D_o for N_2…HCO^+ $\rightarrow N_2 + HCO^+$ and N_2H^+…OC $\rightarrow N_2H^+ + OC$ are ~3500 cm^{-1} and ~5000 cm^{-1}, respectively.